

# NERSC Role in Basic Energy Science Research

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NERSC Director

Requirements Workshop





# NERSC Mission

***Accelerate the pace of scientific discovery for all DOE Office of Science (SC) research through computing and data systems and services.***

***Efficient algorithms***

***+ flexible software***

***+ effective machines***

***→ great computational science.***



# NERSC is the Production Facility for DOE Office of Science

- **NERSC serves a large population**

Approximately 3000 users,  
400 projects, 500 code instances

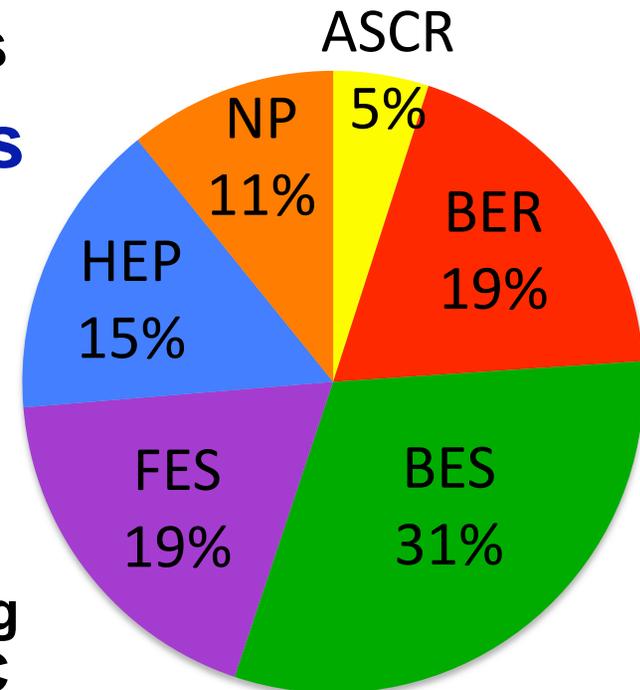
- **Focus on “unique” resources**

- Expert consulting and other services
- High end computing systems
- High end storage systems
- Interface to high speed networking

- **Science-driven**

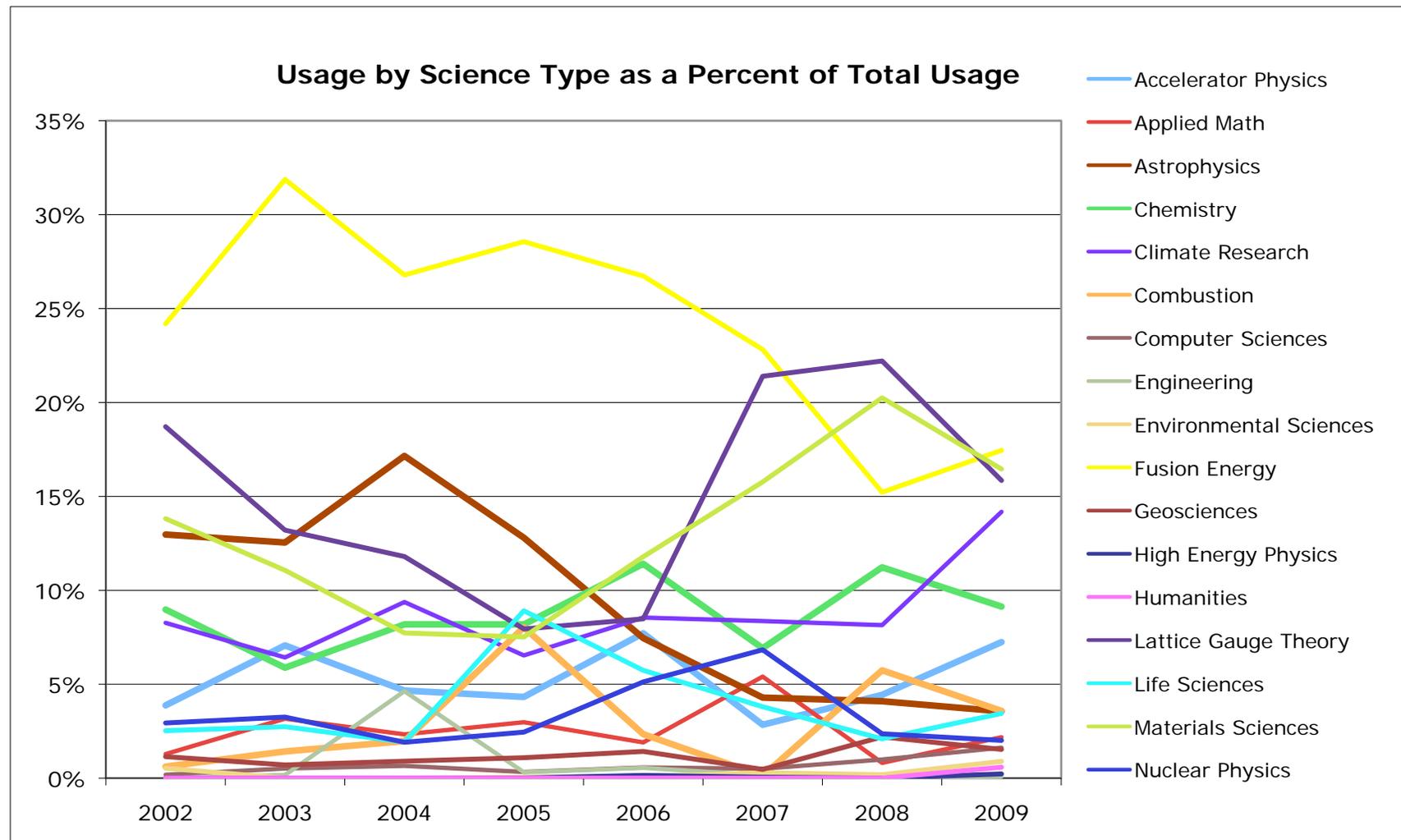
- Machine procured competitively using application benchmarks from DOE/SC
- Allocations controlled by DOE/SC Program Offices to couple with funding decisions

2010 Allocations





# DOE Priorities for NERSC Change Over Time





# ASCR's Computing Facilities

## NERSC at LBNL

- **1000+** users, **100+** projects
- **Allocations:**
  - **80% DOE program manager control**
  - **10% ASCR Leadership Computing Challenge\***
  - **10% NERSC reserve**
- **Science includes all of DOE Office of Science**
- **Machines procured competitively**
- **Introspective security**

## LCFs at ORNL and ANL

- **100+** users **10+** projects
- **Allocations:**
  - **60% ANL/ORNL managed INCITE process**
  - **30% ACSR Leadership Computing Challenge\***
  - **10% LCF reserve**
- **Science limited to largest scale; no limit to DOE/SC**
- **Machines procured through partnerships**
- **Policy-based security**



# NERSC 2010 Configuration

## Large-Scale Computing System

### Franklin (NERSC-5): Cray XT4

- 9,532 compute nodes; 38,128 cores
- ~25 Tflop/s on applications; 356 Tflop/s peak



### Hopper (NERSC-6): Cray XT

- Phase 1: Cray XT5, 668 nodes, 5344 cores
- Phase 2: > 1 Pflop/s peak



### Clusters



### Carver

- IBM iDataplex cluster
- ### PDSF (HEP/NP)
- Linux cluster (~1K cores)

### Cloud testbed

- IBM iDataplex cluster

NERSC Global  
Filesystem (NGF)  
Uses IBM's GPFS  
440 TB; 5.5 GB/s



HPSS Archival Storage

- 59 PB capacity
- 11 Tape libraries
- 140 TB disk cache

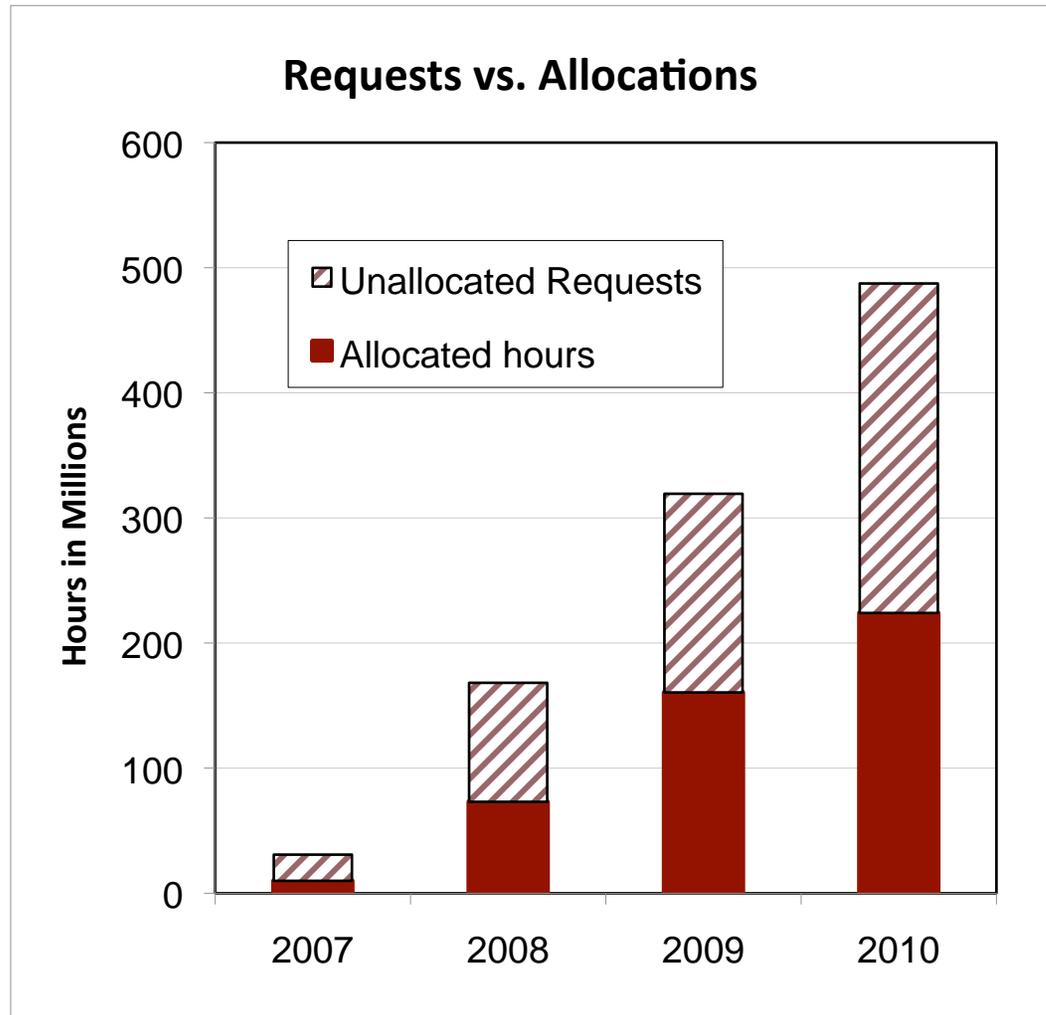


### Analytics / Visualization

- Euclid large memory machine  
- 512 GB shared memory
- GPU testbed  
~40 nodes



# Demand for More Computing



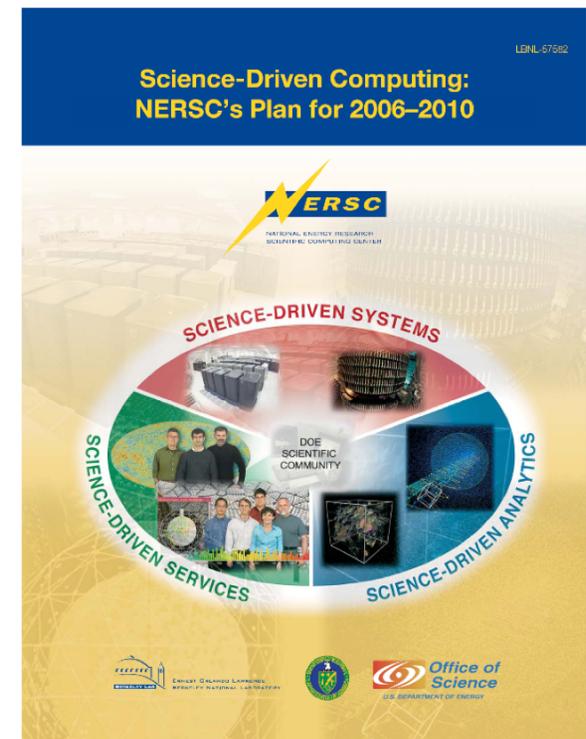
- *Each year DOE users requests ~2x as many hours as can be allocated*
- *This 2x is artificially constrained by perceived availability*
- *Unfulfilled allocation requests amount to hundreds of millions of compute hours in 2010*



# How NERSC Uses Your Requirements

# 2005: NERSC Five-Year Plan

- **2005 Trends:**
  - Widening gap between application performance and peak
  - Emergence of multidisciplinary teams
  - Flood of scientific data
  - (Missed multicore, along with most)
- **NERSC Five-Year Plan**
  - Major system every 3 years
- **Implementation**
  - NERSC-5 (Franklin) and NERSC-6 (underway) + clusters
  - **Question: What trends do you see for 2011-2015?**
    - Algorithms / application trends and other requirements

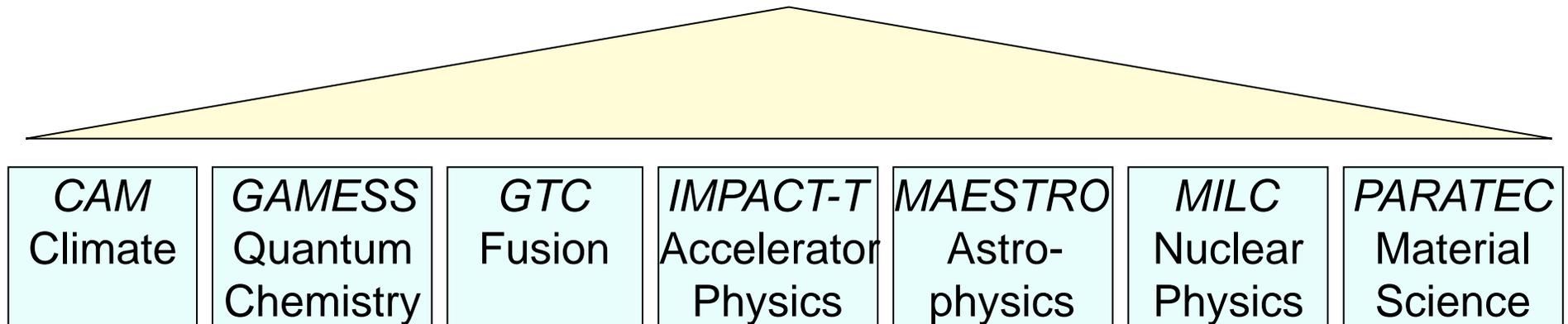




# Applications Drive NERSC Procurements

*Because hardware peak performance does not necessarily reflect real application performance*

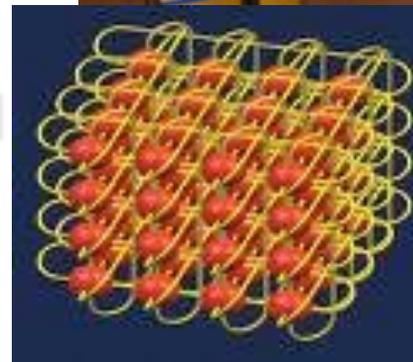
## NERSC-6 “SSP” Benchmarks



- Benchmarks reflect diversity of science and algorithms
- SSP = average performance (Tflops/sec) across machine
- Used before selection, during and after installation
- Question: What applications best reflect your workload?

# NERSC-5 “Franklin”

- **Largest Cray XT4**
  - 102 cabinets
  - 9,740 Quad Core nodes
  - 38,640 CPUs (cores)
  - Novel torus network for large parallel jobs
  - Direct access to parallel filesystem
- **Performance:**
  - 25 Tflop/s of sustained application performance
  - 352 Tflop/s of Peak



**Benjamin Franklin,**  
One of America’s First Scientists,  
performed ground breaking work  
in energy efficiency, electricity,  
materials, climate, ocean currents,  
transportation, health, medicine,  
acoustics and heat transfer.



# NERSC-6 System “Hopper”



Grace Murray Hopper  
(1906-1992)

- Cray system selected competitively:
  - Used application benchmarks from climate, chemistry, fusion, accelerator, astrophysics, QCD, and materials
  - Best application performance per dollar based
  - Best sustained application performance per MW
  - External Services for increased functionality and availability

## Phase 1: Cray XT5

- *In production on 3/1/2010*
- 668 nodes, 5,344 cores
- 2.4 GHz AMD Opteron
- 2 PB disk, 25 GB/s
- Air cooled



## Phase 2: Cray system

- > 1 Pflop/s peak
- ~ 150K cores, 12 per chip
- 2 PB disk, 80 GB/s
- Liquid cooled

4Q09

1Q10

2Q10

3Q10

4Q10

1Q11



U.S. DEPARTMENT OF  
**ENERGY**

Office of  
Science



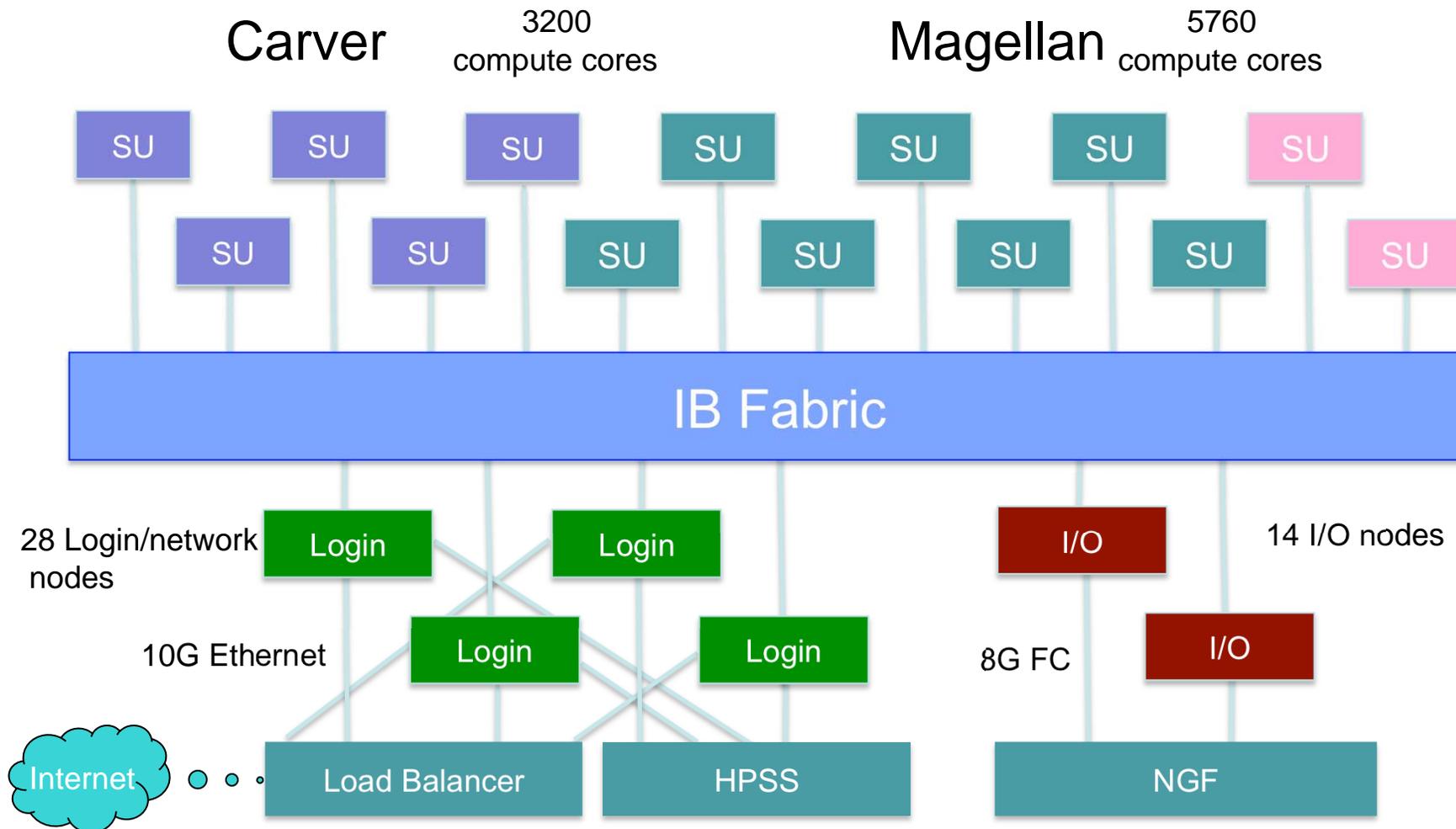


# DOE Explores Cloud Computing

- **DOE's CS program focuses on HPC**
  - No coordinated plan for clusters in SC
- **DOE Magellan Cloud Testbed**
- **Cloud questions to explore:**
  - What are the costs (TCO) of clouds vs other systems?
  - Can a cloud serve DOE's mid-range computing needs?
  - What features (hardware and software) are needed of a "Science Cloud"? Commodity hardware?
  - What requirements do the jobs have (~100 cores, I/O,...)
  - How does this differ, if at all, from commercial clouds which serve primarily independent serial jobs
- **Magellan not a NERSC Program machine**
  - Not allocated in ERCAP; testbed, not production



# Cluster architecture



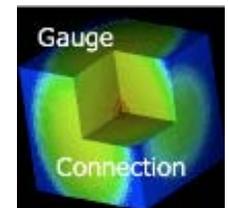
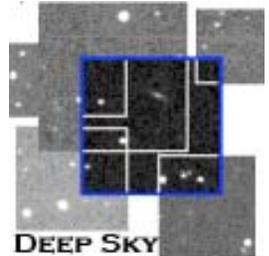


# Reservations at NERSC

- **Reservation service being tested:**
  - Reserve a certain date, time and duration
    - Debugging at scale
    - Real-time constraints in which need to analyze data before next run, e.g., daily target selection telescopes or genome sequencing pipeline
  - At least 24 hours advanced notice
    - <https://www.nersc.gov/users/services/reservation.php>
  - Successfully used for IMG run, Madcap, IO benchmarking, etc.

# Science Gateways at NERSC

- **Create scientific communities around data sets**
  - Models for sharing vs. privacy differ across communities
  - Accessible by broad community for exploration, scientific discovery, and validation of results
  - Value of data also varies: observations may be irreplaceable
- **A science gateway is a set of hardware and software that provides data/services remotely**
  - Deep Sky – “Google-Maps” of astronomical image data
    - Discovered 140 supernovae in 60 nights (July-August 2009)
    - 1 of 15 international collaborators were accessing NGF data through the SG nodes 24/7 using both the web interface and the database.
  - Gauge Connection – Access QCD Lattice data sets
  - Planck Portal – Access to Planck Data
- **Building blocks for science on the web**
  - Remote data analysis, databases, job submission



# Visualization Support

*Petascale visualization:* Demonstrate visualization scaling to unprecedented concurrency levels by ingesting and processing unprecedentedly large datasets.

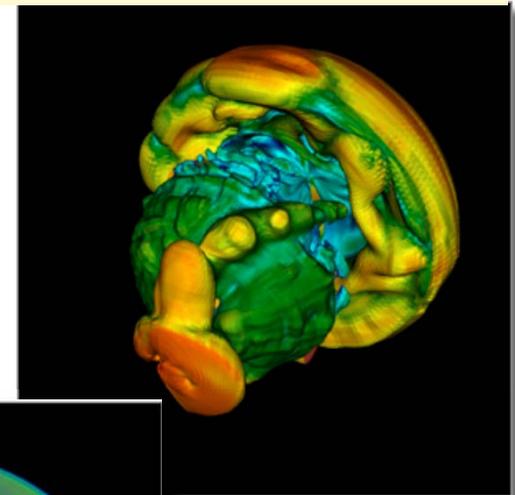
*Implications:* Visualization and analysis of Petascale datasets requires the I/O, memory, compute, and interconnect speeds of Petascale systems.

*Accomplishments:* Ran VisIt SW on 16K and 32K cores of Franklin.

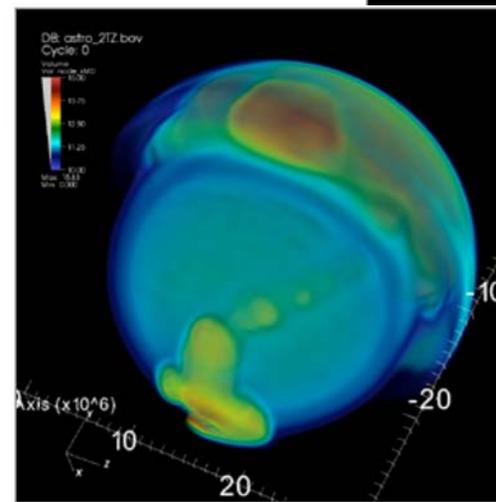
- First-ever visualization of two *trillion* zone problem (TBs per scalar); data loaded in parallel.
- Petascale visualization

Plots show 'inverse flux factor,' the ratio of neutrino intensity to neutrino flux, from an ORNL 3D supernova simulation using CHIMERA.

b



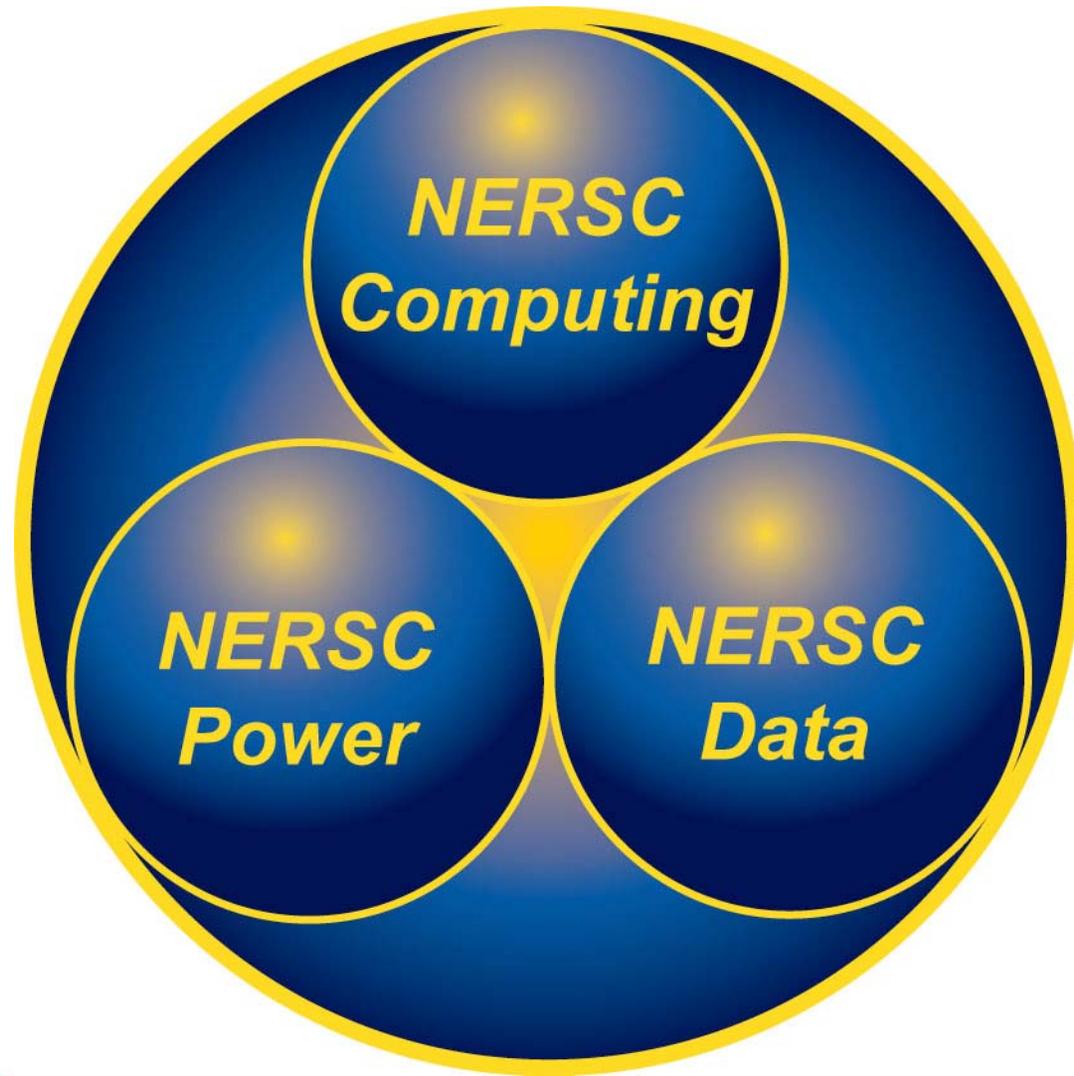
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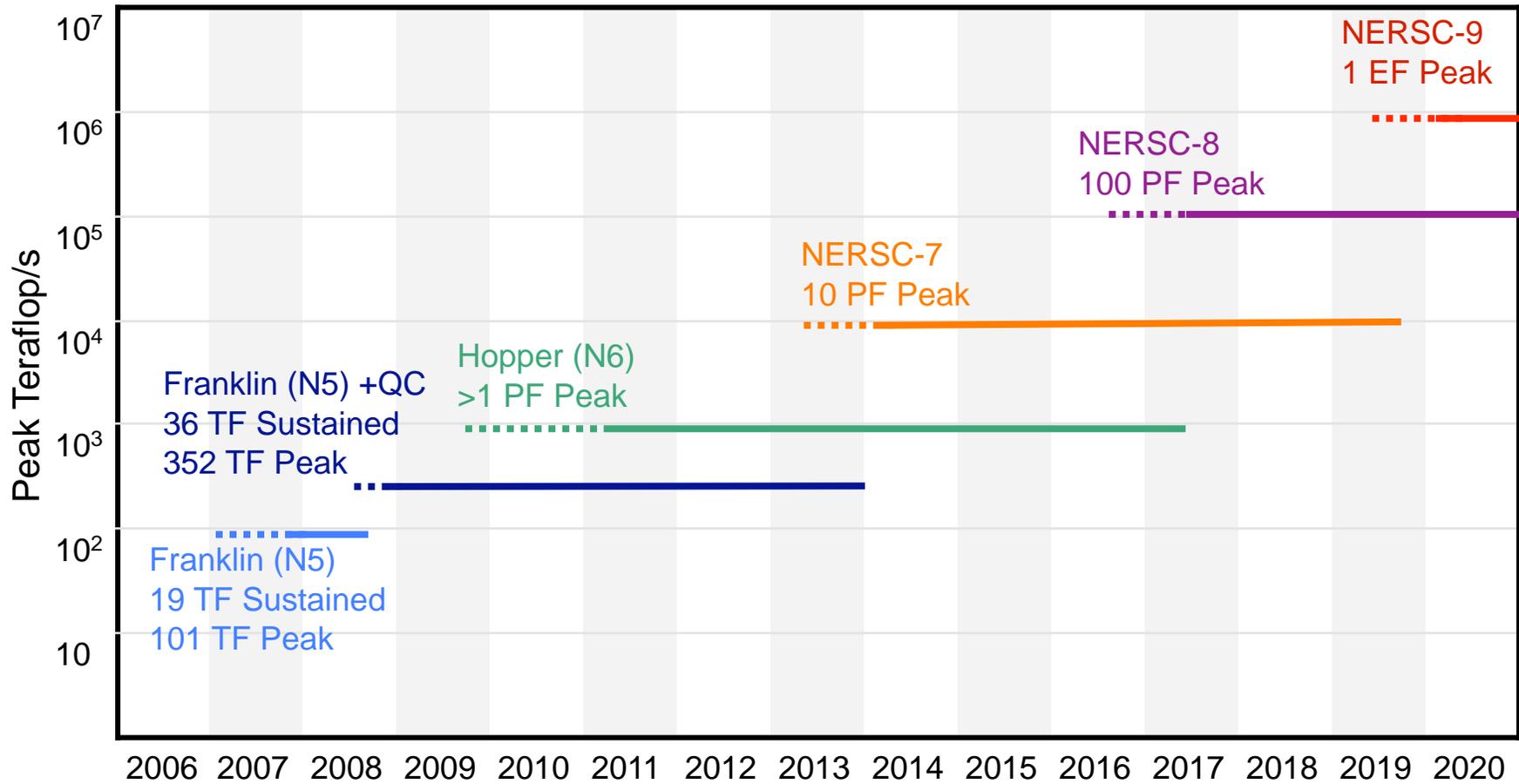
Isocontours (a) and volume rendering (b) of two trillion zones on 32K cores of Franklin.



# Requirements Drive NERSC's Long-Term Vision



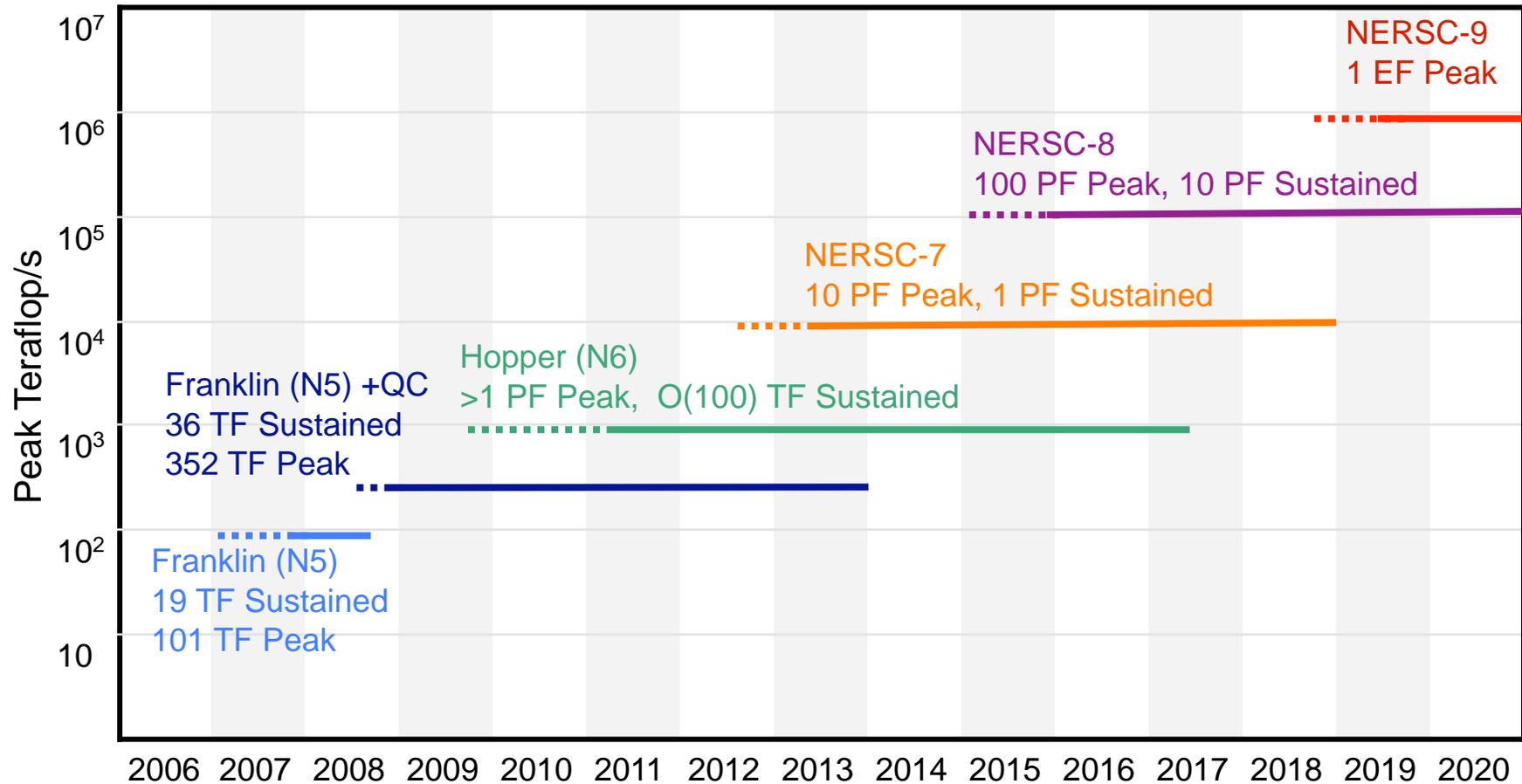
# NERSC System Roadmap



- **Goal is two systems on the floor at all times**
- **Systems procured by sustained performance**



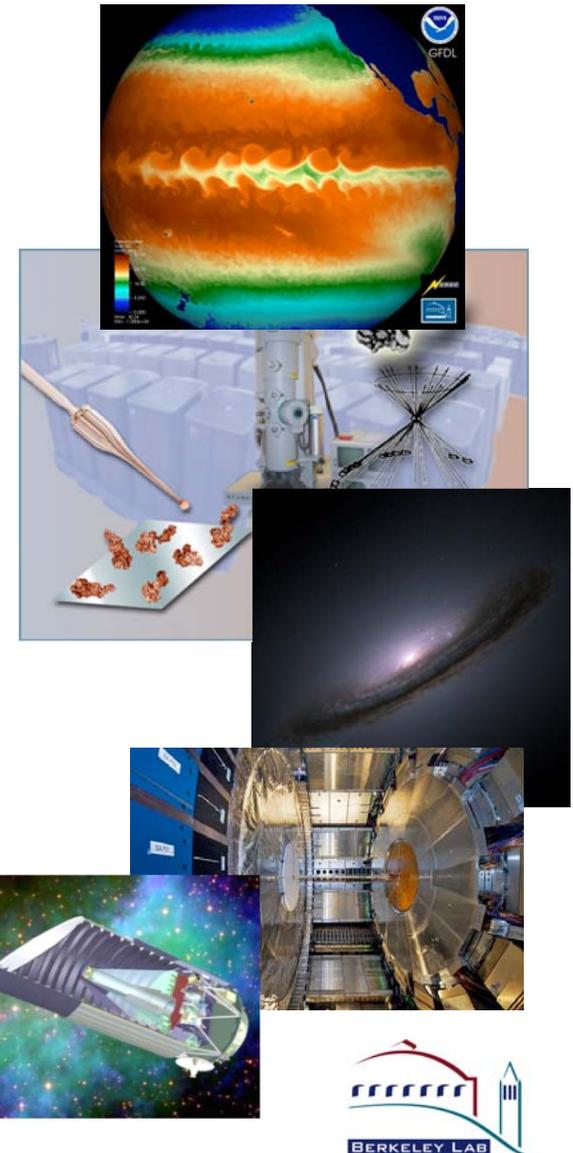
# NERSC Aggressive Roadmap



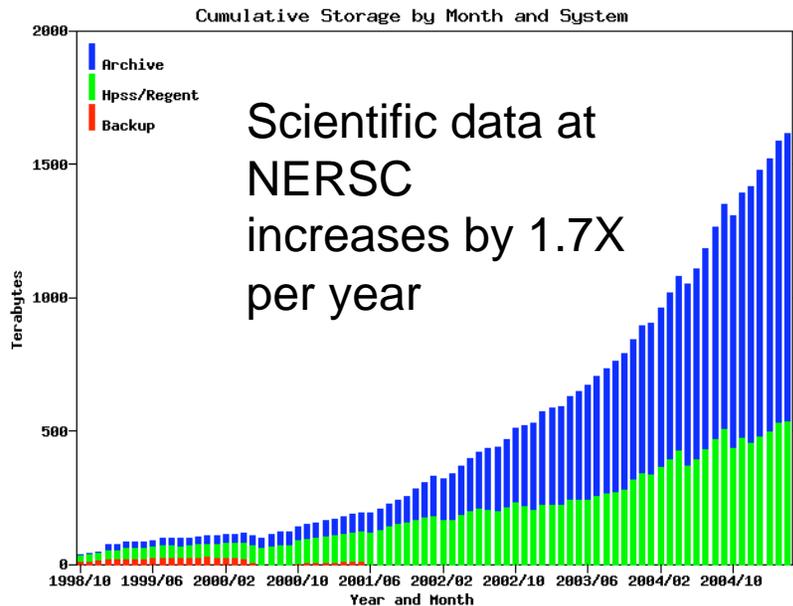
- Assume machines are well-balanced so that typical DOE application performance is 5-10% of peak
- Does DOE science justify 10x more capability by 2013? 100x by 2015?

# Data Driven Science

- **Scientific data sets are growing exponentially**
  - Ability to generate data is exceeding our ability to store and analyze
  - Simulation systems and some observational devices grow in capability with Moore's Law
- **Petabyte (PB) data sets will soon be common:**
  - *Climate modeling*: estimates of the next IPCC data is in 10s of petabytes
  - *Genome*: JGI alone will have .5 petabyte of data this year and double each year
  - *Particle physics*: LHC is projected to produce 16 petabytes of data per year
  - *Astrophysics*: LSST and others will produce 5 petabytes/year
- **Create scientific communities with "Science Gateways" to data**

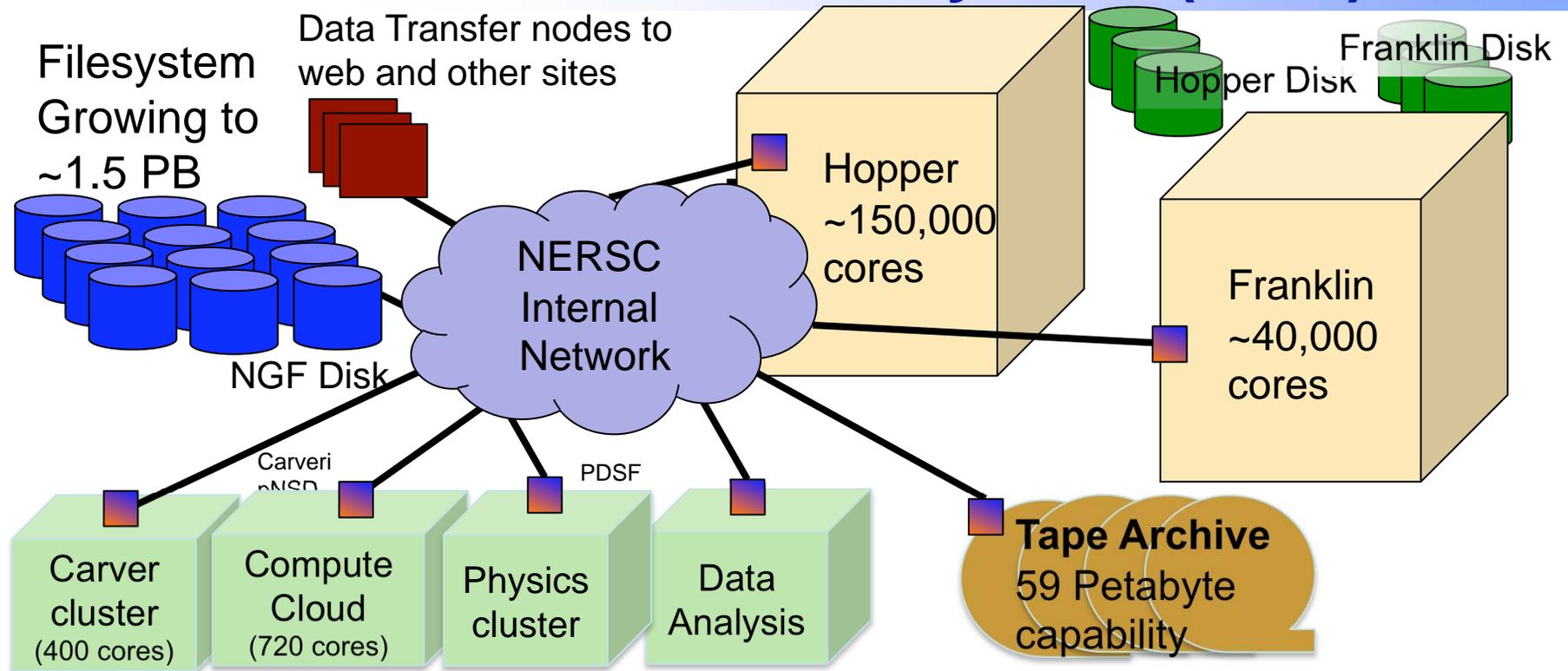


# Tape Archives: Green Storage



- **Tape archives are important to efficient science**
  - 2-3 orders of magnitude less power than disk
  - Requires specialized staff and major capital investment
  - NERSC participates in development (HPSS consortium)
- **Questions: What are your data sets sizes and growth rates?**

# NERSC Architecture with NERSC Global Filesystem (NGF)



- NERSC has a modest number of “commodity systems”
- Mostly specialized science systems for compute, disk storage (parallel filesystems), and tape archives

# Communication Services

*Since 2007, NERSC is a net data importer. In support of our users, it is important that we take on a lead role in improving intersite data transfers.*

- **Systems and software typically tuned only within a site**
- **Technical, social, and policy challenges abound:**
  - High performance transfer software has too many options → hard to use.
  - Systems designed for computation can have bottlenecks in data transfers
  - Systems at different sites often often have incompatible versions of transfer software.
  - Trying to maintain security exceptions (firewall holes) for all the systems and software at each site was impossible.
- **... and the list goes on.**
- **NERSC established Data Transfer Nodes (DTNs).**
  - Reduced transfer time of 30 TB from 30+ days to 2 days
  - We formed a working group with experts at the three labs and ESNet

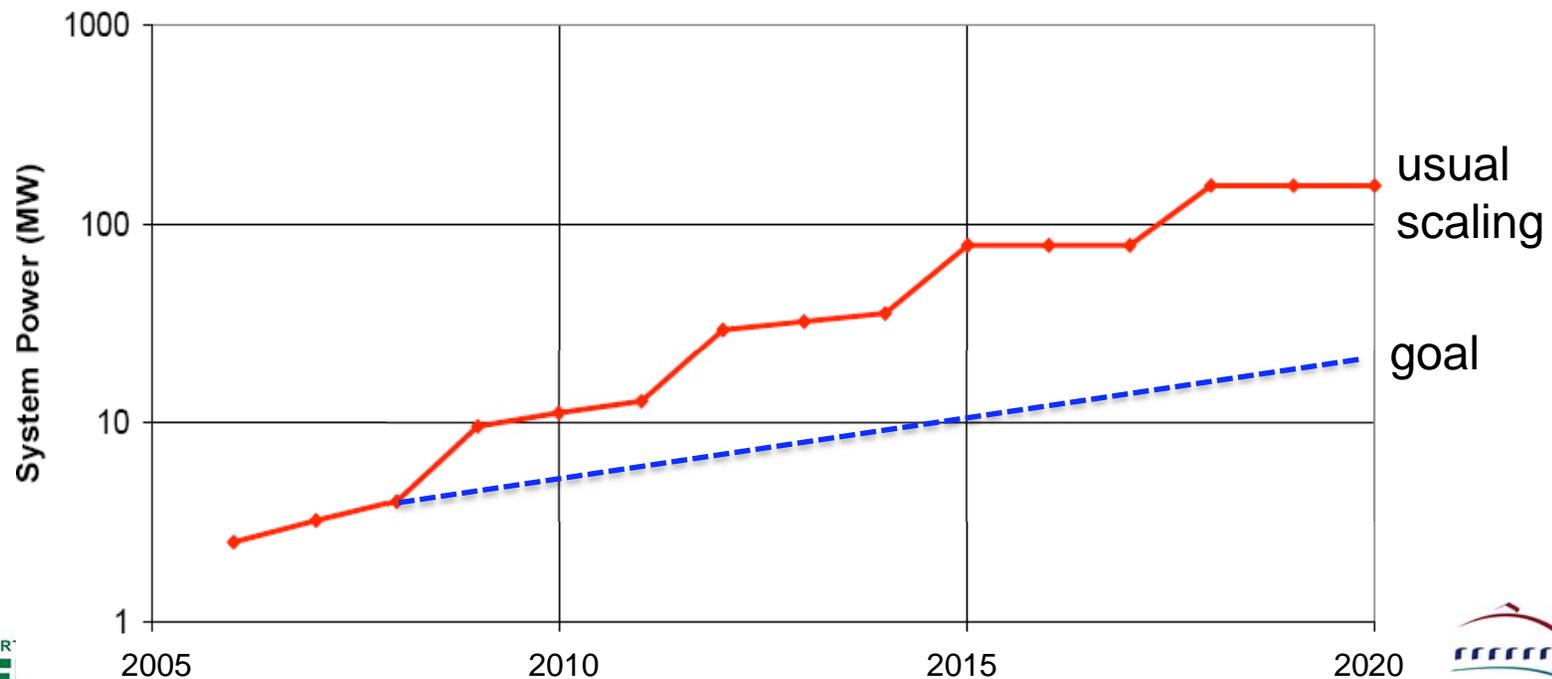
<http://www.nersc.gov/nusers/systems/DTN>

<http://fasterdata.es.net>

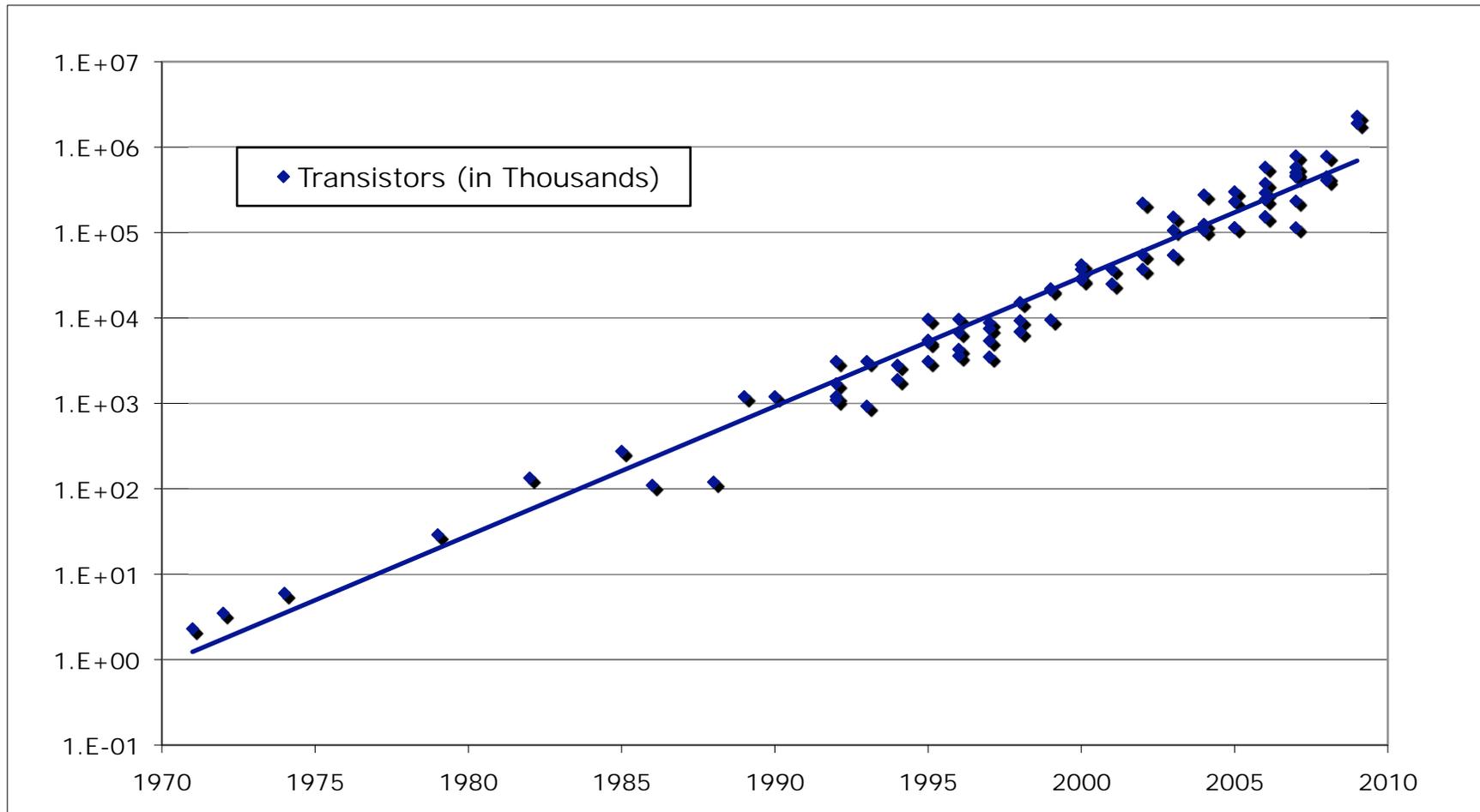


# Energy Efficiency is Necessary for Computing

- Systems have gotten about 1000x faster over each 10 year period
- 1 petaflop ( $10^{15}$  ops) in 2010 will require 3MW  
→ 3 GW for 1 Exaflop ( $10^{18}$  ops/sec)
- DARPA committee suggested 200 MW with “usual” scaling
- Target for DOE is 20 MW in 2018

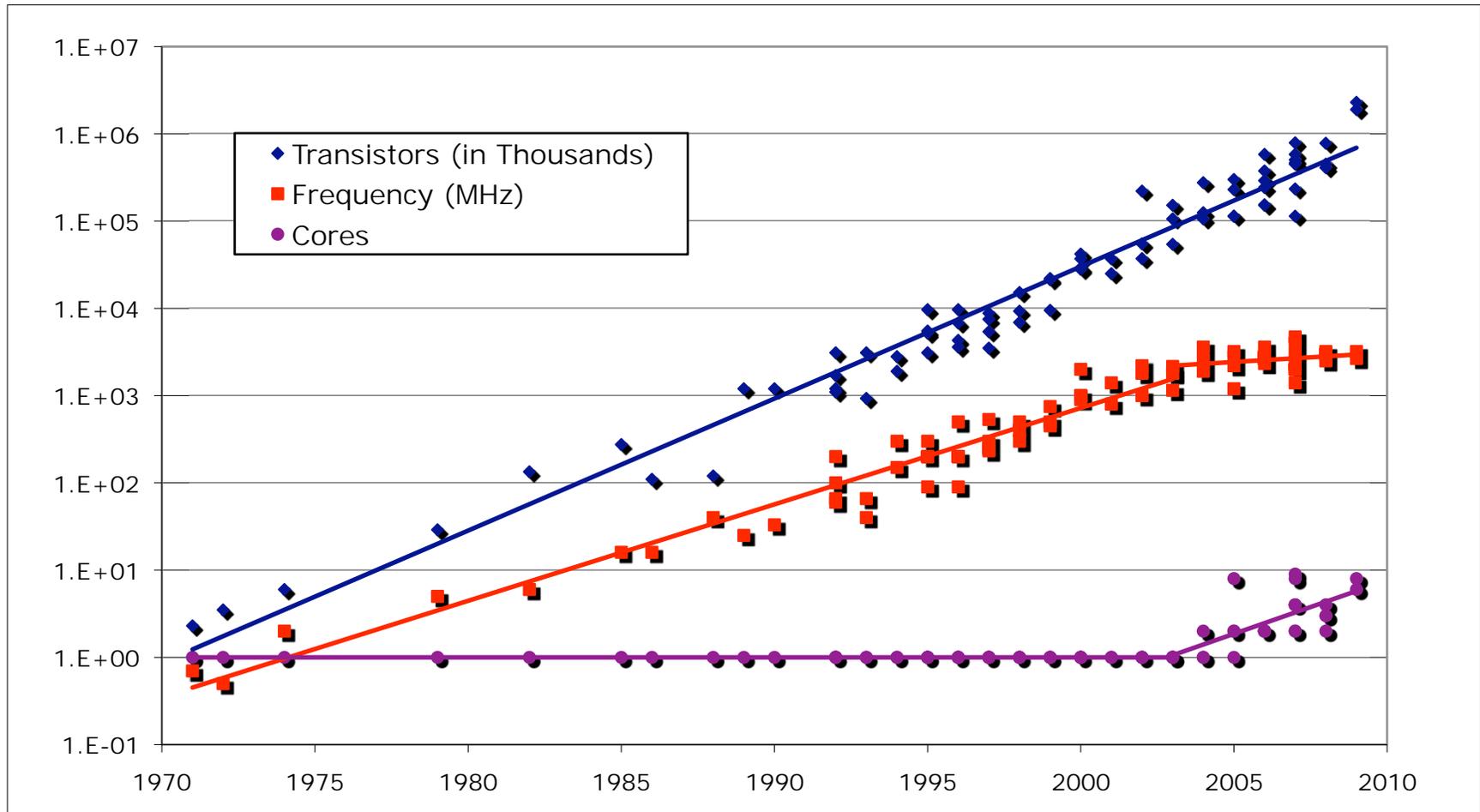


# Moore's Law is Alive and Well



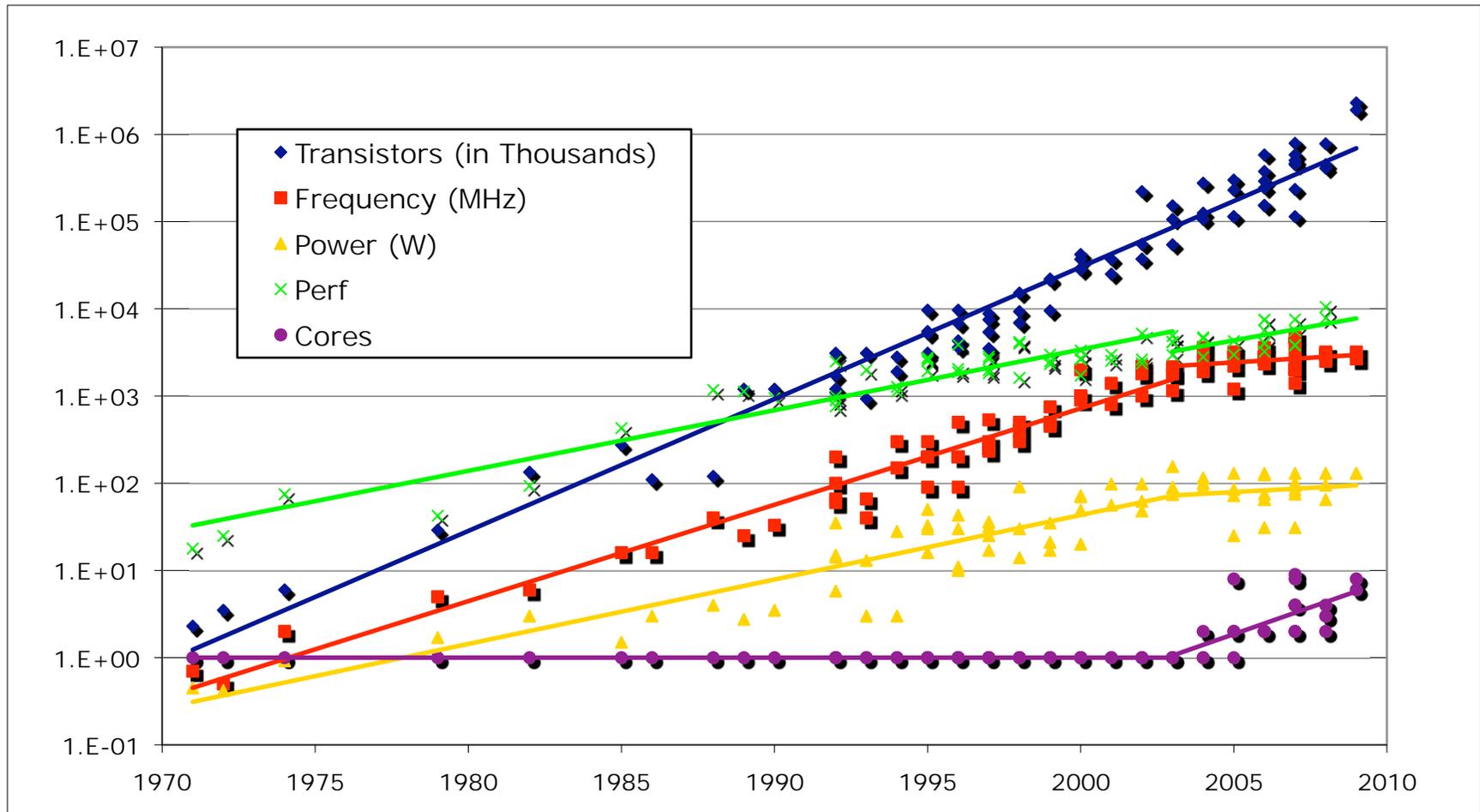
Data from Kunle Olukotun, Lance Hammond, Herb Sutter,  
Burton Smith, Chris Batten, and Krste Asanović

# But Clock Frequency Scaling Replaced by Scaling Cores / Chip



Slide Source: Kathy Yelick. Data from Kunle Olukotun, Lance Hammond, Herb Sutter, Burton Smith, Chris Batten, and Krste Asanović

# Performance Has Also Slowed, Along with Power (Root Cause)

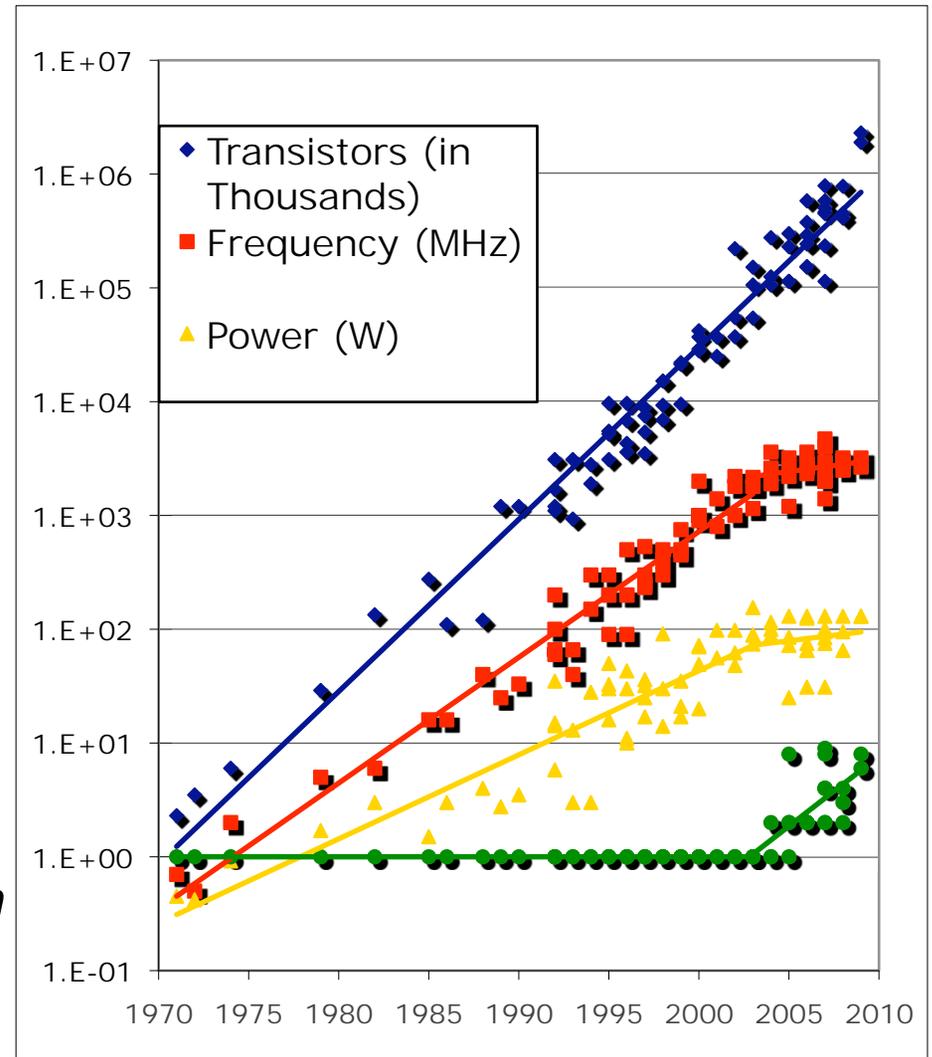


Slide Source: Kathy Yelick. Data from Kunle Olukotun, Lance Hammond, Herb Sutter, Burton Smith, Chris Batten, and Krste Asanović



# NERSC Goal Usable Exascale in 2020

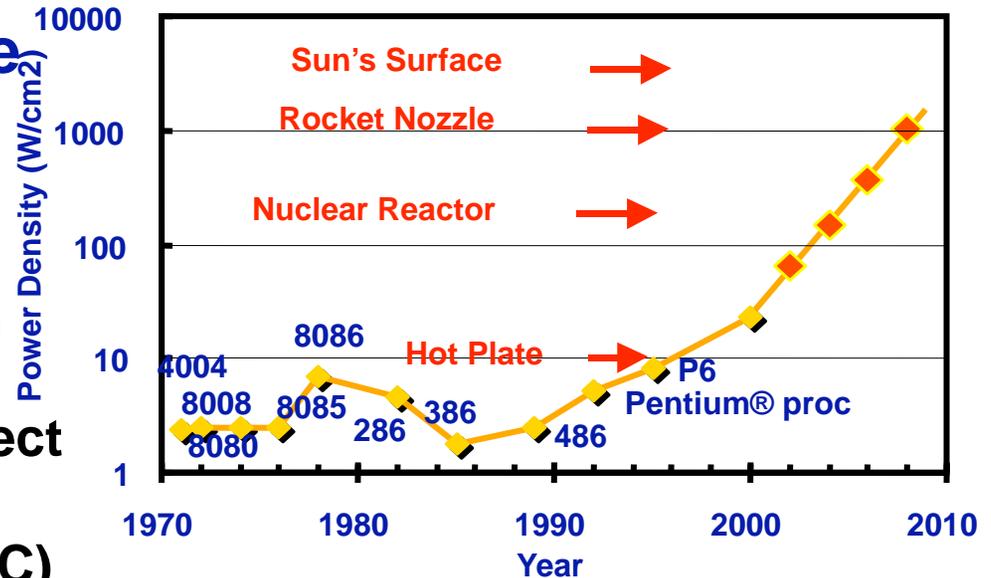
- Computational scaling changed in 2004
- Problems also for laptops, handhelds, data centers
- Parallelism on-chip brings algorithms, programming into question
- ***NERSC: Programmable, usable systems for science***
  - 1) *Energy efficient designs*
  - 2) *Facilities to support scale for both high and mid scale*



# Parallelism is “Green”

- **Concurrent systems are more power efficient**

- Dynamic power is proportional to  $V^2fC$
- Increasing frequency ( $f$ ) also increases supply voltage ( $V$ ) → cubic effect
- Increasing cores increases capacitance ( $C$ ) but only linearly



- **High performance serial processors waste power**

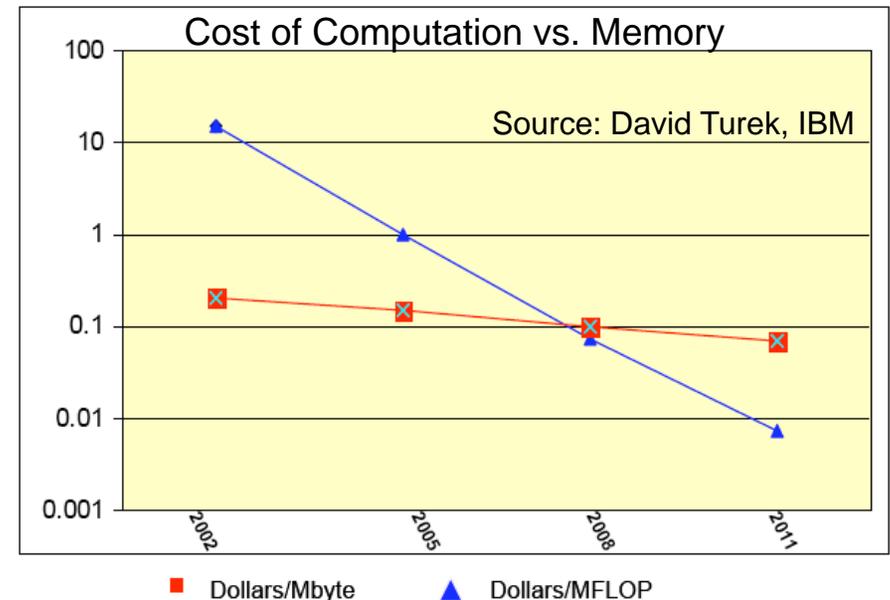
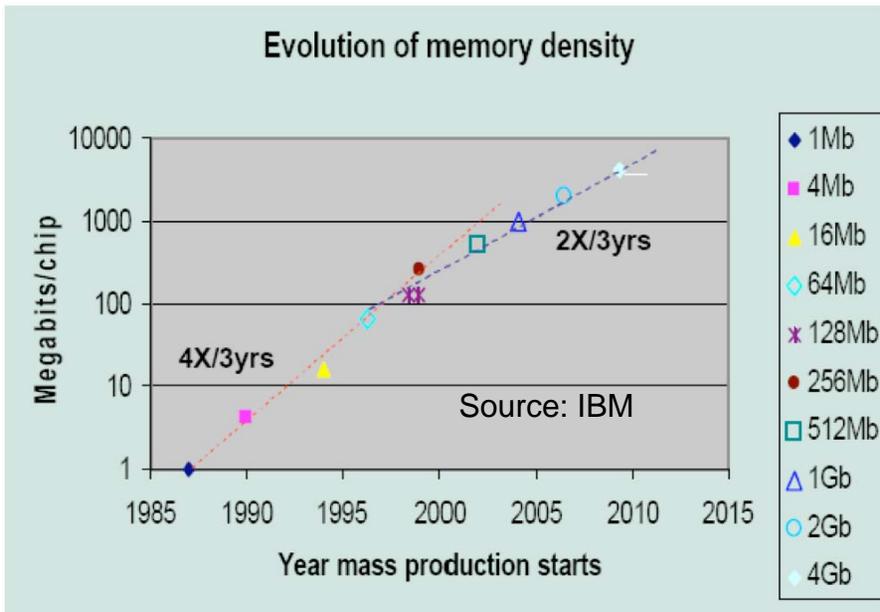
- Speculation, dynamic dependence checking, etc. burn power
- Implicit parallelism discovery

- **Question: *Can you double the concurrency in your algorithms and software every 2 years?***

# Technology Challenge

Technology trends against a constant or increasing memory per core

- Memory density is doubling every three years; processor logic is every two
- Storage costs (dollars/Mbyte) are dropping gradually compared to logic costs



The cost to sense, collect, generate and calculate data is declining much faster than the cost to access, manage and store it

Question: *Can you double concurrency without doubling memory?*



# Hardware and Software Trends

- **Hardware Trends**
  - Exponential growth in explicit on-chip parallelism
  - Reduced memory and memory bandwidth per core
  - Heterogeneous computing platforms (e.g., GPUs)
  - As always, hardware is largely driven by non HPC markets
- **Software Response**
  - Need to express more explicit parallelism
  - New programming models on chip: MPI + X
  - Increased emphasis on strong scaling
  - No more serial code scaling from hardware
- **What we want**
  - Understand your requirements and help craft a strategy for transitioning to a hardware and programming environment solution



# Basic Energy Science at NERSC



# QMC Electronic Structure

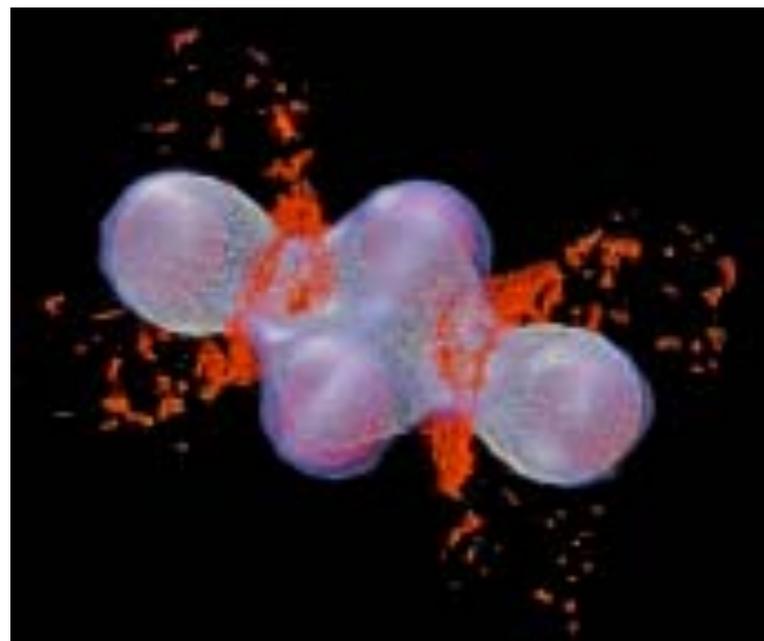
**Objective:** Develop Quantum Monte Carlo (QMC) methods to stochastically solve many-body electronic structure problems.

**Implications:** Accurately predict or explain chemical phenomena where other methods fail or aren't applicable.

**Accomplishments:** Developed hybrid QMC / Molecular Mechanics formalism.

- Obtained interaction energy of a 2-water cluster treating one H<sub>2</sub>O quantum mechanically and other classically; prelude to effort to find much sought-after electron binding energy in (H<sub>2</sub>O)<sub>n</sub>.
- Studied series of Li clusters in different charge states to obtain energies for cluster growth, charge, and discharge in interactions with graphene.
- ZORI scales to 32K cores on Franklin

**W. Lester, UCB**



Cluster of four Li atoms and electron cloud (red) as calculated by ZORI on NERSC's Cray XT4

# Chemistry: Improving Catalysis

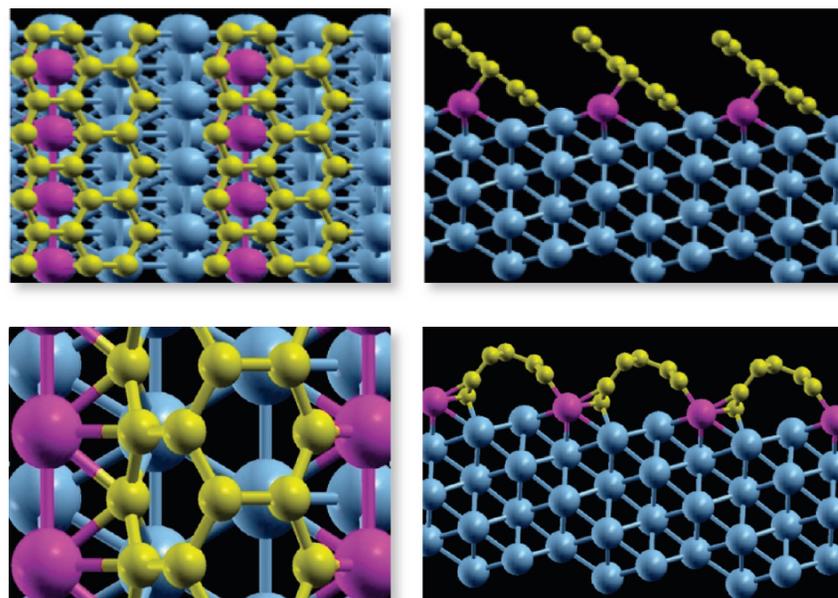
**Objective:** First-principles studies to develop better catalytic processes.

**Implications:** Improved power sources such as lithium-ion batteries, fuel cells.

**Accomplishments:** DFT studies of catalyzed single-walled carbon nano-tube growth on Cobalt nano-particles.

- Predict most stable adsorption sites.
- Carbon atoms form curved & zigzag chains in various orientations – some are likely precursors to graphene.
- Showed strong preference for certain metal sites.
- Next step is to investigate growth on chiral surfaces
- Modest parallelism

**P. Balbuena, Texas A&M**



*Simulation showing carbon atom chains (yellow) on cobalt surfaces (blue & pink).*

*J. Phys. Chem. C, Sept, 2009 Cover Story*

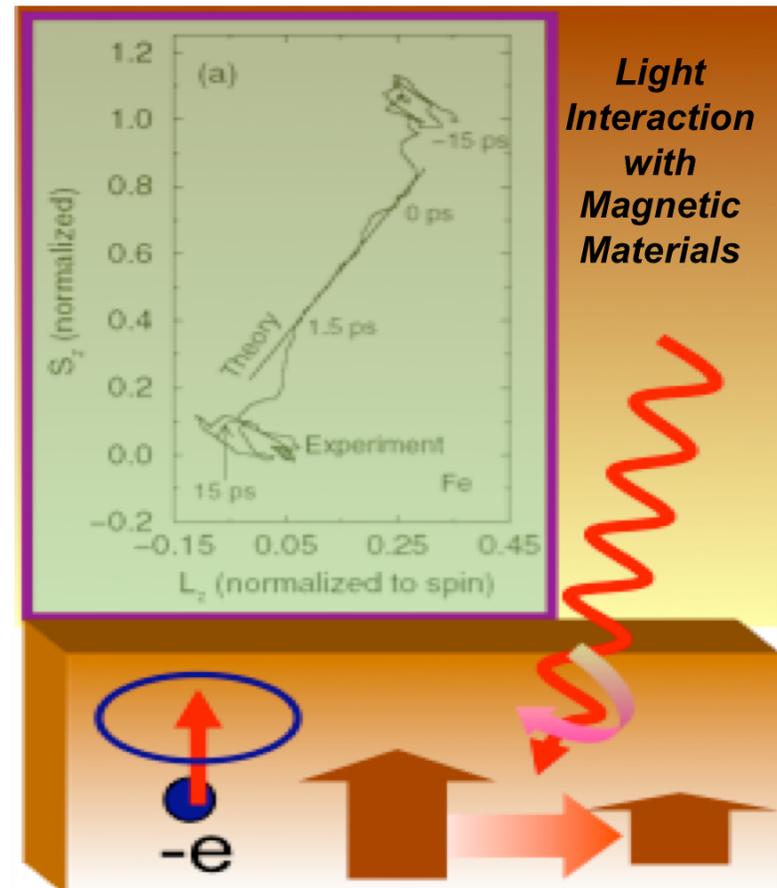
**Objective:** Explore ultrafast optical switching of nanoscale magnetic regions.

**Implications:** Potential for laser operated hard drives, 1000s of times faster than today's technology.

**Accomplishments:** First-principles, time- & spin-dependent DFT study using locally-designed code on laser-irradiated Ni.

- Discovered that light leverages the crystal structure to transfer spin of electrons to higher orbit.
- Study is the first to clearly demonstrate that this phenomenon is a relativistic effect connected with electron spin.
- Discovery matches experiment and can guide synthesis of new materials.
- Used over 1.5M hours in 2009; 2,800 cores

## G. Zhang (Indiana St)



*J. Appl. Phys.* (2008)

# Finding Hidden Oil / Gas Reserves

**Objective:** Apply new, highly rigorous, massively parallel, 3-D imaging techniques to create geophysical maps of hydrocarbon reservoirs in unprecedented levels of detail.

**Implications:** New detection abilities and exploration savings by revealing where hydrocarbon deposits reside, even when covered by ocean over a mile deep and several more miles of rock below the ocean. Can also be used for locating potential sites for CO<sub>2</sub> sequestration.

**Accomplishments:** Has already provided insight into complex geology of Campos Basin, a petroleum rich area near Brazil.

**NERSC:** Code developed on Franklin.

- Algorithms can run on O(10,000) cores; designed to scale well beyond. Runs on Franklin routinely use 4,000-8,000 cores.

**G. Newman, M. Commer  
(LBNL)**

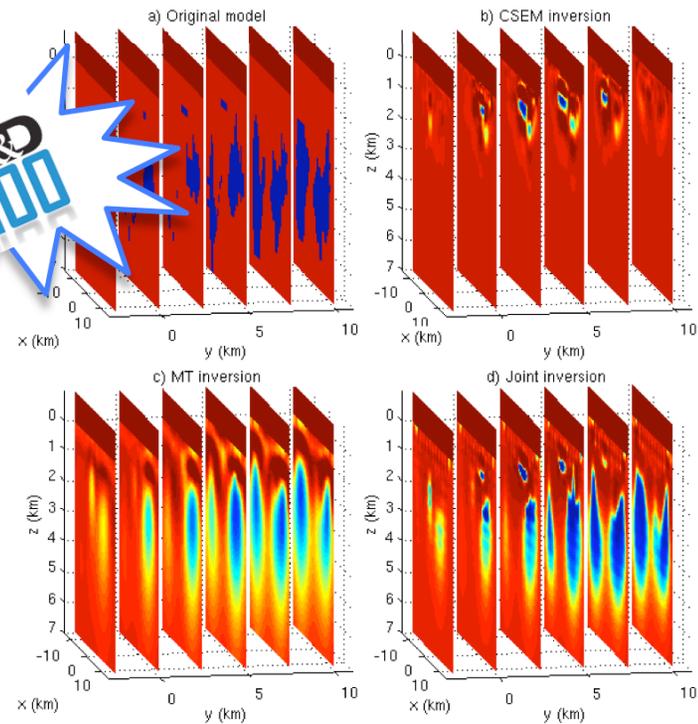


Image improvement resulting from the method. Original data (a), controlled-source electromagnetic method (CSEM) alone (b), magnetotellurics (MT) alone (c) and combined CSEM and MT (d).

# Graphene as the Ultimate Membrane for Gas Separation

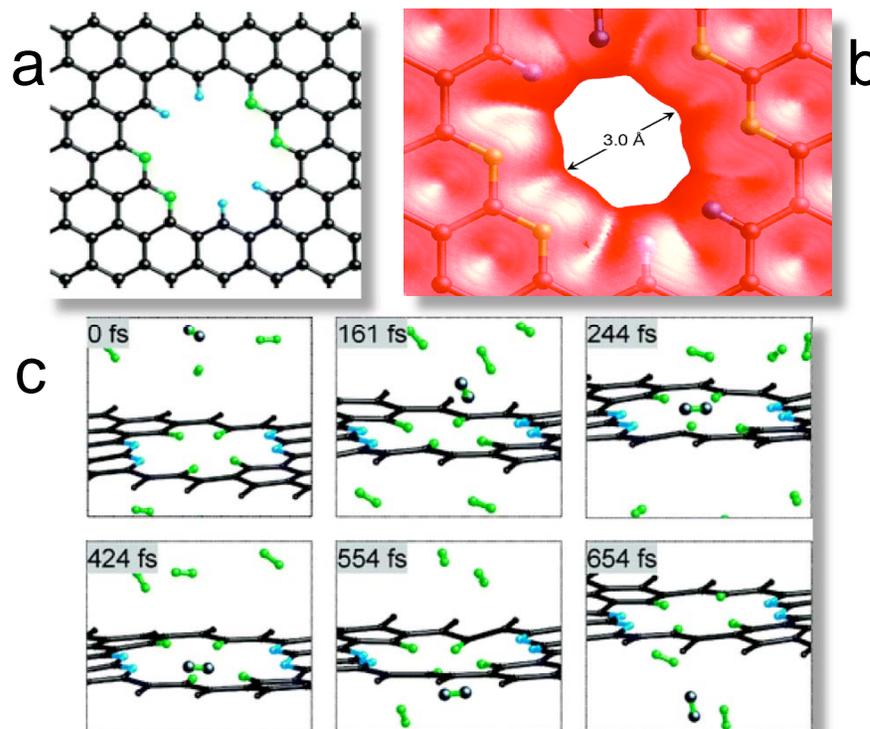
**Objective:** Study permeability, selectivity of graphene with custom sub-nanometer pores using *ab initio* DFT and vdW DF.

**Implications:** Potentially lower energy costs for purification and production of key industrial gases such as H<sub>2</sub> and methane.

**Accomplishments:** Such pores exhibit extremely high selectivity, presenting a formidable barrier for CH<sub>4</sub> but easily surmountable for H<sub>2</sub>.

- Results suggest that graphene may be superior to traditional membranes.
- Could have widespread impact on numerous energy and technological applications, including carbon sequestration, fuel cells and gas sensors.

**D. Jiang (PI), V. Cooper, S. Dai (ORNL)**



Nitrogen-functionalized pore in graphene (a), electron density isosurface (b), and snapshots of H<sub>2</sub> diffusing through the pore from NERSC first principles molecular dynamics simulations.

# Restructuring Catalyst Surfaces

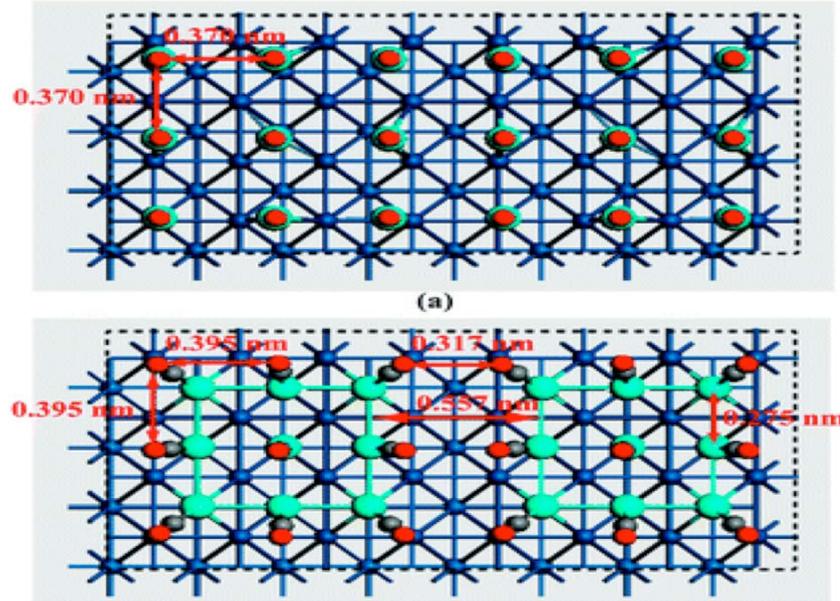
**Objective:** Use simulation to understand the ability of surfaces to restructure under the influence of gaseous adsorbates.

**Implications:** Revealing the arrangement of metal atoms that form at active sites will yield increased understanding of heterogeneous catalysis mechanisms.

**Accomplishments:** DFT studies at NERSC show that CO molecules bind to small Pt nanoclusters on the catalyst surface.

- The nanoclusters seem to maximize bonding of more CO molecules.
- VASP reveals the stabilization energy gained by cluster formation and suggests the atomic arrangement.
- Formation of small metallic clusters opens a new avenue for understanding catalytic activity under high pressures.

## Lin-Wang Wang (LBNL)



(top) Starting geometry of CO and Pt atoms. (bottom) After relaxation to minimize energy in the DFT calculation, two (3 × 3) clusters form. Dark blue circles represent Pt atoms in the slab layers; light blue circles represent Pt atoms at the surface. Red and gray circles represent oxygen and carbon atoms, respectively.

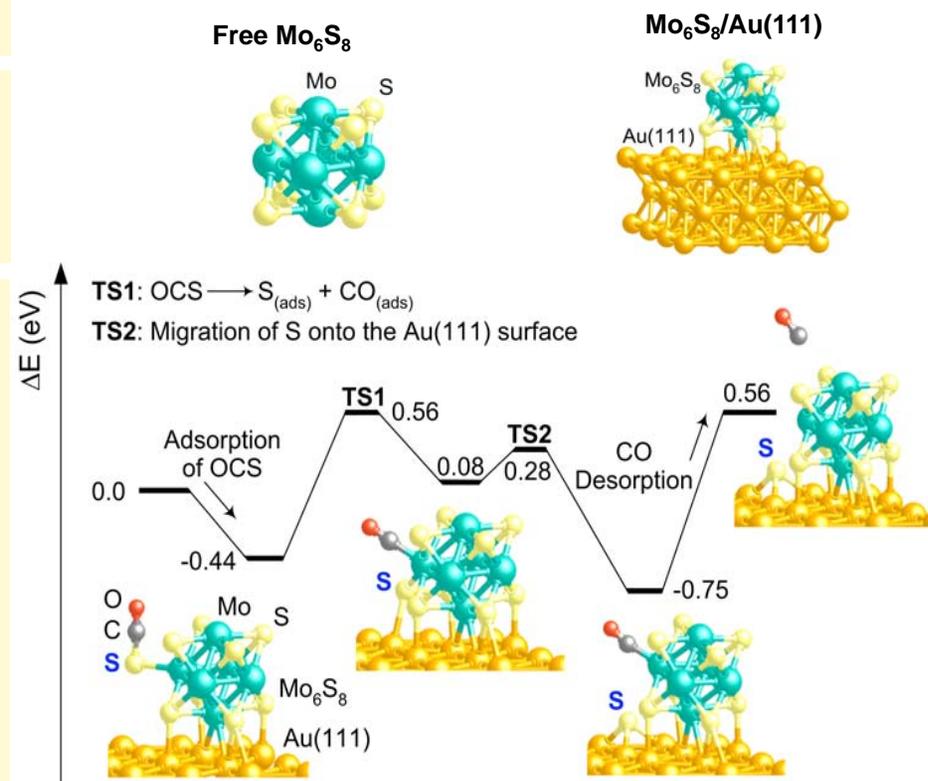
**Objective:** Study small metal clusters supported on nanoparticles to understand heterogeneous catalysis; help design improved catalysts.

**Implications:** Better hydrodesulphurization in power plants; possible conversion and use of non-conventional fuels, e.g., MeOH.

**Accomplishments:** DFT calculations and state-of-the-art cluster beam studies provide insight into the reaction mechanism of catalytic activity of molybdenum-sulfur clusters on gold surfaces.

- Help identify intermediates along the catalytic reaction pathway.
- Used over 700K hours in 2009
- Special ORNL/NERSC version of VASP

**P. Liu (BNL)**



Potential energy profile for the interaction of Carbonyl Sulfide (OCS) on  $\text{Mo}_6\text{S}_8/\text{Au}(111)$

*J. Phys. Chem. A (2009)*

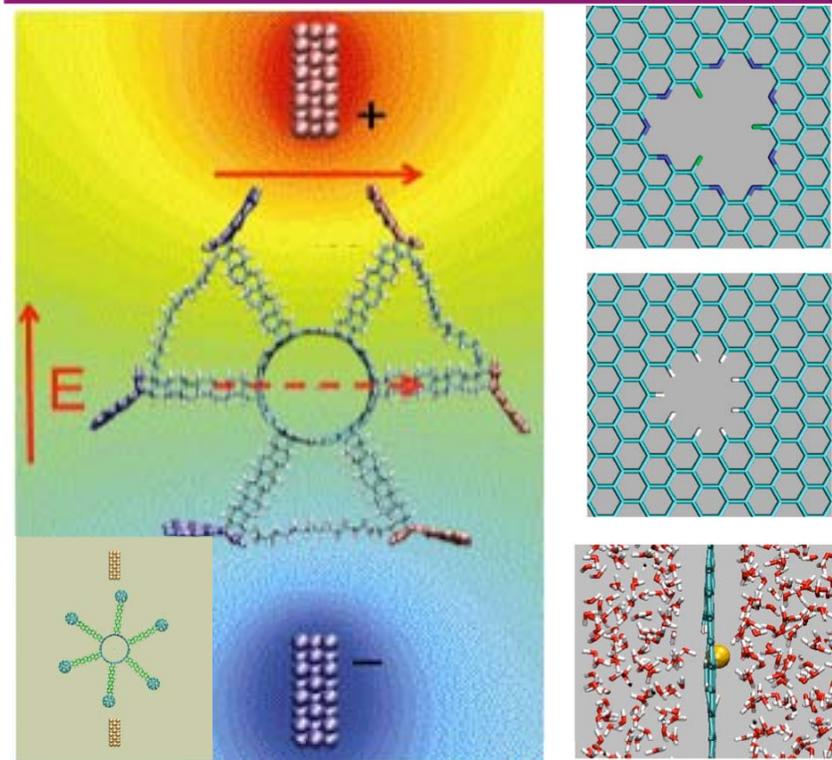
**Objective:** design, simulate and help realize nanoscale molecular transport systems.

**Implications:** Possible use in drug delivery, advanced sieves, desalination.

**Accomplishments:** Simulations of nanomotors, nanotubes, micelles, and custom-designed nanopores using Molecular Dynamics.

- Showed that
  - Electron tunneling can drive nano-scale motors used in nanopropellers.
  - Functionalized graphene-based nanopores can serve as ionic sieves.
  - Nanodroplets can be dragged on the surface of carbon nanotubes.
  - NAMD on Franklin; >250K hour in 2009

**Petr Král, UIC**



Click here

Left: Nanomotor rotates in presence of electric field; Right: two example highly-selective nanosieves – only certain ions pass across.

*Phys Rev Lett., J Chem Phys., and JACS, (2008)*

# Novel Material Simulations

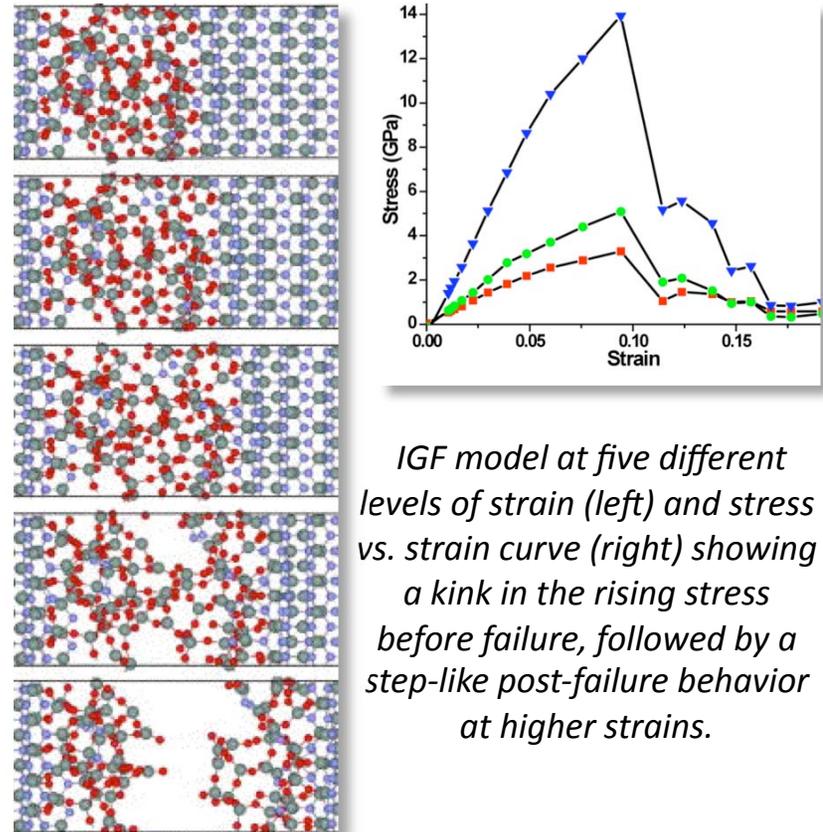
**Objective:** Electronic structure studies of complex ceramic materials with outstanding thermal & electrical properties.

**Implications:** Connection of atomic-scale characteristics with engineering mechanics and elucidation of properties not available by any other method.

**Accomplishments:** VASP DFT study of mechanical response and failure behavior of intergranular glassy films (IGFs) in Silicon Nitrides.

- Stress/strain relationship explained by fundamental electronic structure of the model.
- May be used to guide future material designs that enhance selective properties.
- Used >2.5M hours on Franklin in 2009

**W. Ching, UMKC**



*IGF model at five different levels of strain (left) and stress vs. strain curve (right) showing a kink in the rising stress before failure, followed by a step-like post-failure behavior at higher strains.*

*Appl. Phys. Lett. (2009)*

# Molecular Geochemistry

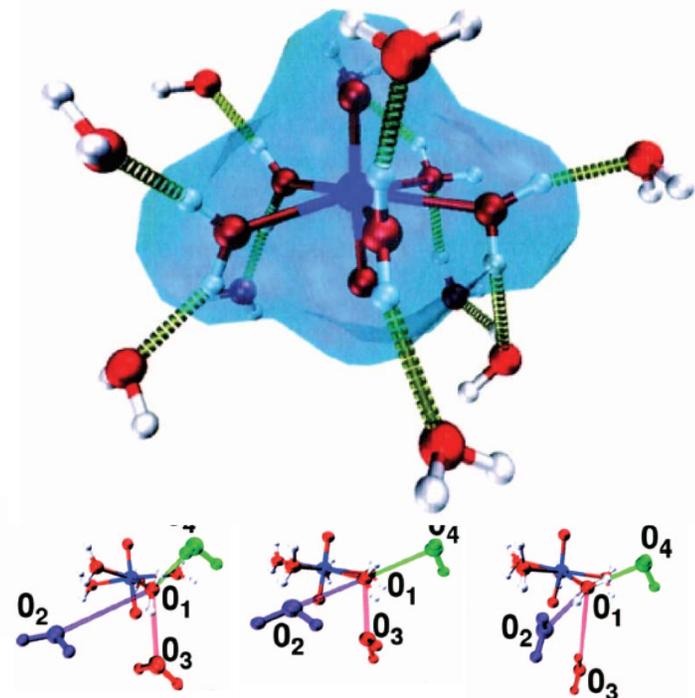
**Objective:** Accurate structural studies of contaminants in solution.

**Implications:** Predict long-term viability of nuclear waste containment strategies.

**Accomplishments:** Two different NWChem *ab initio*-DFT analyses of Uranium Oxide ion ( $\text{UO}_2^{2+}$ ), one with 64  $\text{H}_2\text{O}$  molecules for 22 ps and one with 122 waters for 9 ps.

- Extremely-demanding simulations due to large # of  $\text{H}_2\text{O}$  molecules and long integration times.
- Results help explain X-Ray spectra but also reveal additional structural features.
- Also provides NWChem to other NERSC users

**E. Bylaska, A. Felmy, PNNL**



*First-principles molecular dynamics simulation of 2<sup>nd</sup> hydration shell surrounding  $\text{UO}_2^{2+}$  with 3 intermediate dissociative structures.*

*J Chem Phys (2008)*

# Catalysis for Higher Fuel Cell Efficiency

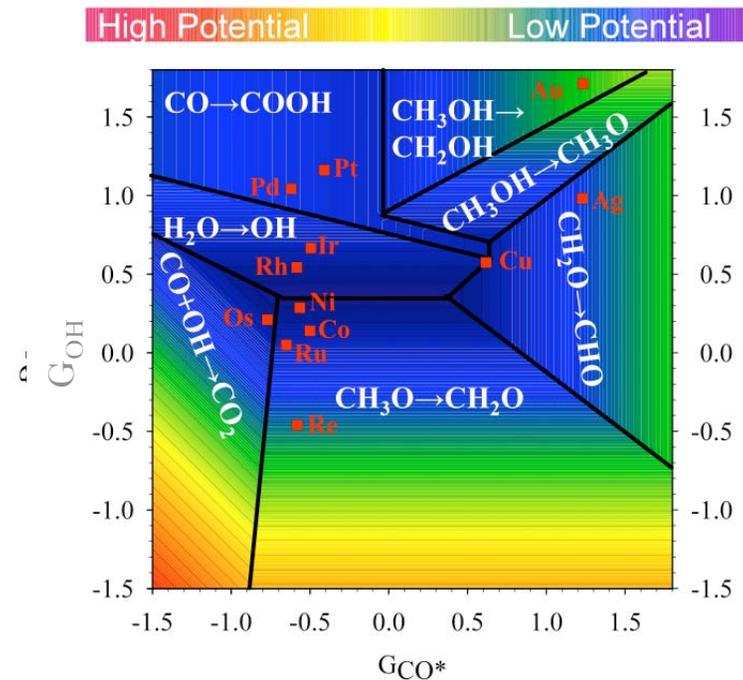
**Objective:** Identify and evaluate catalytic surfaces aimed at improving the efficiency of Direct Methanol Fuel Cells (DMFCs).

**Implications:** Lower power, more efficient and economical DMFCs have potential applications in powering mobile phones and laptop batteries and as an alternatives to current hydrogen fuel cell technology.

### Accomplishments:

- Used DFT to develop an electrochemical model to evaluate catalytic surfaces for methanol oxidation.
- Model helps identify properties of an 'ideal' catalyst and allows screening of novel systems that may be better and cheaper than current technology.
- Significant effort by NERSC Services for special VASP version used here

**M. Mavrikakis (U.Wisc)**



*This figure shows the potential determining steps from the DFT calculations. It helps predict the lowest possible potential of a fuel cell, which is directly related to the efficiency of the catalyst.*



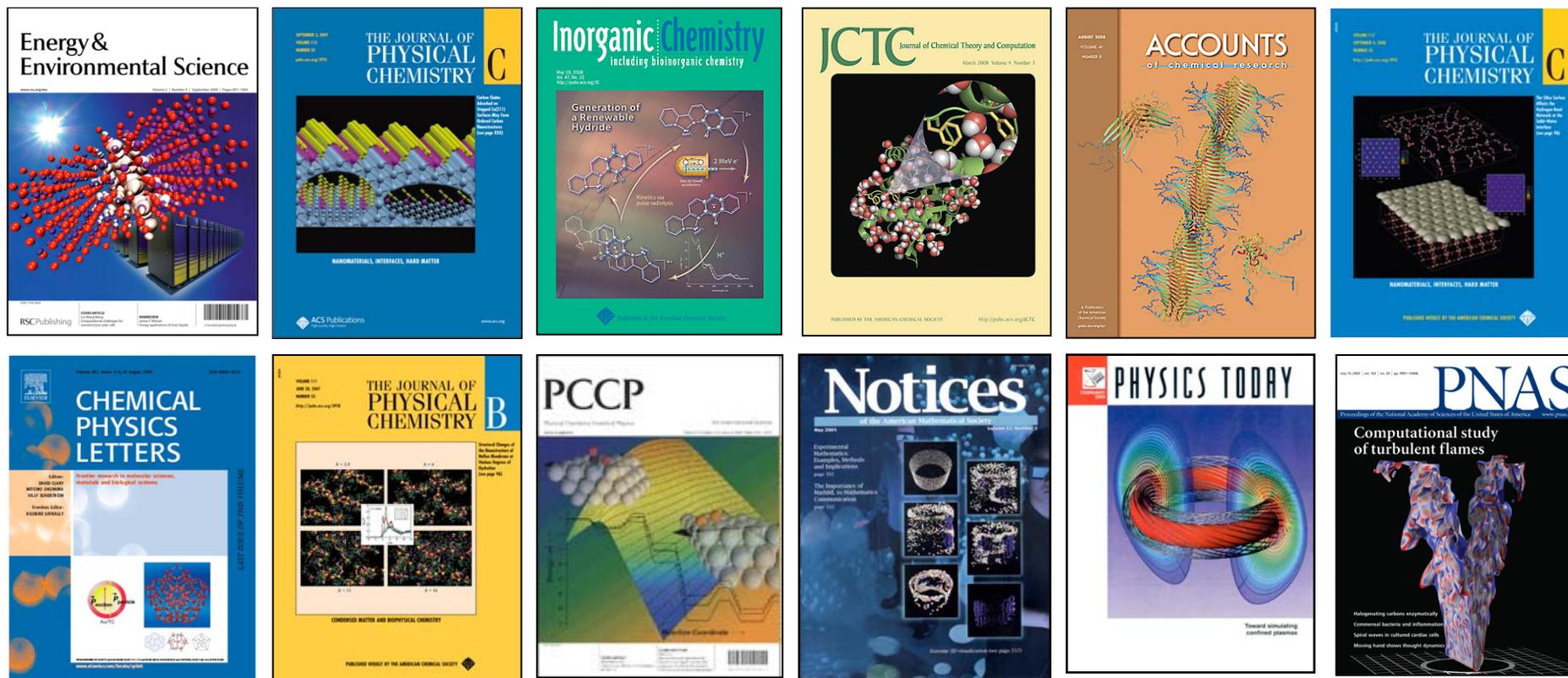
# NISE: NERSC Initiative for Scientific Exploration

- **INCITE program was created at NERSC:**
  - Focused computing and consulting resources
  - Became the allocation mechanism for the LCFs
- **NISE program at NERSC (started in 2009)**
  - Programming techniques for multicore and scaling in general
  - Science problems near breakthrough (encourage high risk/payoff)
  - <http://www.nersc.gov/nusers/accounts/NISE.php>
- **AY09 (10/1/09 through 01/11/10) ~20M Franklin hours made available to existing NERSC projects; ~6.9M to BES**
  - Elasticity of b-DNA Models; Metallic Alloy Fatigue Fracture; Minimum Free Energy Paths/Profiles of Protein Conformational Changes; Diamondoid-Nanoparticle Enhanced Organometallic Surfaces; Organic Photovoltaics, AIMBPT; MeOH Reformation; Nanocluster Energy Landscape; Graphene Bilayer Electronic Device; Sec Translocase Transmembrane Channel
- **See also ASCR's ALCC Program:**  
<http://www.er.doe.gov/ascr/Facilities/ALCC.html>

# Conclusions

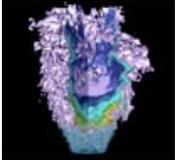
- **NERSC requirements**
  - Qualitative requirements shape NERSC functionality
  - Quantitative requirements set the performance
    - “What gets measure gets improved”
- **Goals:**
  - Your goal is to make scientific discoveries
    - Articulate specific scientific goals and implications for broader community
  - Our goal is to enable you to do science
    - Specify resources (services, computers, storage, ...) that NERSC could provide with quantities and dates

# Cover Stories from NERSC Research



NERSC is enabling new science in all disciplines,  
with about *1,500 refereed publications* per year

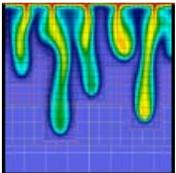
# About the Cover



**Low swirl burner combustion simulation.** Image shows flame radical, OH (purple surface and cutaway) and volume rendering (gray) of vortical structures. Red indicates vigorous burning of lean hydrogen fuel; shows cellular burning characteristic of thermodynamically unstable fuel. Simulated using an adaptive projection code. Image courtesy of John Bell, LBNL.



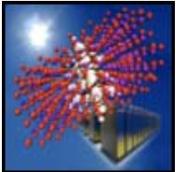
**Hydrogen plasma density wake produced by an intense, right-to-left laser pulse.** Volume rendering of current density and particles (colored by momentum orange - high, cyan - low) trapped in the plasma wake driven by laser pulse (marked by the white disk) radiation pressure. 3-D, 3,500 Franklin-core, 36-hour LOASIS experiment simulation using VORPAL by Cameron Geddes, LBNL. Visualization: Gunther Weber, NERSC Analytics.



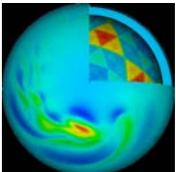
**Numerical study of density driven flow for CO<sub>2</sub> storage in saline aquifers.** Snapshot of CO<sub>2</sub> concentration after convection starts. Density-driven velocity field dynamics induces convective fingers that enhance the rate by which CO<sub>2</sub> is converted into negatively buoyant aqueous phase, thereby improving the security of CO<sub>2</sub> storage. Image courtesy of George Pau, LBNL



**False-color image of the Andromeda Galaxy created by layering 400 individual images captured by the Palomar Transient Factory (PTF) camera in February 2009.** NERSC systems analyzing the PTF data are capable of discovering cosmic transients in real time. Image courtesy of Peter Nugent, LBNL.



**The exciton wave function (the white isosurface) at the interface of a ZnS/ZnO nanorod.** Simulations performed on a Cray XT4 at NERSC, also shown. Image courtesy of Lin-Wang Wang, LBNL.



**Simulation of a global cloud resolving model (GCRM).** This image is a composite plot showing several variables: wind velocity (surface pseudocolor plot), pressure (b/w contour lines), and a cut-away view of the geodesic grid. Image courtesy of Professor David Randall, Colorado State University.